Ethanone, 1-(2,4-dihydroxyphenyl)-89-84-9 | DTXSID4058998

89-84-9	DTXSID4058998	

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 8.76e-01

Global applicability domain: Inside

Local applicability domain index: 6.37e-01

Confidence level: 6.84e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Benzenediol, 2,6-dimethyl-

Measured: 1.00 Predicted: 1.24

Image not found

Methylhydroquinone
Measured: 0.91

Predicted: 1.05

Image not found

2-Hydroxyphenylacetic acid

Measured: 0.85 Predicted: 9.03e-01

Image not found

3-Hydroxyphenylacetic acid

Measured: 0.85
Predicted: 9.01e-01